

On the absence of conduction electrons in the antiferromagnetic part of the phase-separated states in magnetic semiconductors *

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Abstract

We have calculated the energies of the phase-separated states for degenerate antiferromagnetic semiconductors including the possibility of the existence of conduction electrons in the antiferromagnetic part of the phase-separated states. It is demonstrated that, at $T = 0$, the minimum energy corresponds to a droplet phase with absence of electrons in the antiferromagnetic part.

1 Introduction

Degenerate antiferromagnetic semiconductors are obtained by strongly doping antiferromagnetic semiconductors (e.g., *EuTe* or lanthanum manganites). Over a concentration range of doping impurities, the ground state of these compounds will be a mixture of antiferromagnetic (AF) and ferromagnetic (FM) phases [1, 2, 3]. Starting from a pure compound and doping, it is found that the ground state is AF and non-conducting up to some conduction electron concentration, driven by impurities, n_d , for which the homogeneous state turns to be unstable against phase separation. The ground state becomes then inhomogeneous with a simply connected AF phase and a multiply

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connected FM phase. The exact geometry of the multiply connected phase is of fractal nature. On increasing the doping, a geometric transition takes place in which the topology of the sample changes due to percolation of the FM phase. Now, the ground state corresponds to a multiply connected AF phase and a simply connected FM one. The doping concentration at which this transition occurs is denoted by n_T . At this point an important change in the conductivity is expected, because the material becomes a conductor. On a further increase of doping, a certain concentration, n_u , exists at which this phase-separated state starts to be unstable and the sample becomes again homogeneous but now a FM. Transitions between these phases are also observed by varying magnetic field and temperature [4].

The physical reason for having a phase-separated state in an antiferromagnetic semiconductor is the dependence of the energy of the charge carriers that appear on doping on the magnetic order of the lattice. The charge carrier energy is lower if they move in a FM region. Therefore, by interaction with the spin system in the lattice, they are able to change its magnetic order, creating FM micro-regions and become trapped in them. In a degenerate magnetic semiconductor this is a cooperative phenomenon: a number of carriers are self-trapped in the same FM micro-region reducing the energy per carrier necessary to create it. When the carrier concentration is high enough, the phase-separated state turns out to be stable. It must be stressed that our calculation is valid only in the case of a degenerate semiconductor, i.e. over the range of conduction electron density in which this collective behaviour of the carriers appears. The micro-region contains a high number of conduction electrons. No individual (isolated) ferrons (magnetic polarons) exists over this range of concentrations. Unfortunately, there is no means of calculate n_d accurately, simply it must be defined as the density from which these micro-regions contain a “high” number of conduction electrons.

Within the Vonsovsky s-d model and using a variational procedure to calculate the energies of the different phases, Nagaev shows that the phase-separated state was the ground state for degenerate antiferromagnetic semiconductors over a certain range of doping. One of the assumptions of the calculation is the absence of conduction electrons in the AF part of the phase-separated state (see the reference [1] for a review). In this article we modified the calculations in [1] to allow for the presence of conduction electrons in the AF part of phase-separated state and we shown that the energy minimum is encountered when all the conduction electrons are in the FM phase.

2 The Hamiltonian of the system

Our starting point is the Hamiltonian of the generalized Vonsovsky s-d model:

$$\begin{aligned}
 H = & \sum E_{\vec{k}} a_{\vec{k}\sigma}^\dagger a_{\vec{k}\sigma} - \frac{A}{N} \sum \vec{S}_{\vec{h}} \vec{s}_{\sigma\sigma'} \exp[i(\vec{k} - \vec{k}')\vec{g}] \\
 & \times a_{\vec{k}\sigma}^\dagger a_{\vec{k}'\sigma'} - \frac{1}{2} \sum I(\vec{g} - \vec{f}) \vec{S}_{\vec{g}} \vec{S}_{\vec{f}} + H_C
 \end{aligned} \tag{1}$$

where $a_{\vec{k}\sigma}^\dagger$, $a_{\vec{k}\sigma}$ are the creation and destruction operators of a conduction electron with quasi-momentum \vec{k} and spin projection σ , $\vec{S}_{\vec{g}}$ is the operator of the core spins of the magnetic ions (d-spins) with number \vec{g} , $\vec{s}_{\sigma\sigma'}$ are the Pauli matrices and N is the total number of unit cells in the crystal. The crystal structure is assumed to be simple cubic, the d-spin magnitude being S . In the case of that the conduction electrons move on the magnetic ions the label \vec{h} in the second term of equation (1) is equal to \vec{g} . But in the case of the electron moving on a non-magnetic atom then \vec{h} corresponds to the nearest magnetic neighbors of this ion and summation is carried over them. The term bilinear in the d-spin operators will be called the exchange Hamiltonian, though in reality it corresponds to the super-exchange interaction between magnetic ions. The term H_C describes the Coulomb energy of interaction of the conduction electrons with each other and with ionized impurities. The charge of the latter, compensating the charge of the conduction electrons, is assumed to be distributed uniformly over the sample (the jellium model).

The main parameters in the Vonsovsky s-d model are $W = 2zt$, the carriers band-width, AS the exchange energy between conduction electrons and magnetic ions (s-d exchange energy) and zIS^2 the exchange energy between magnetic ions (d-d exchange energy). $I < 0$ is the exchange integral between first-nearest neighbors magnetic ions. The smallest parameter is the d-d exchange energy, which is of the order of magnitude of Néel temperature of the pure compound (without doping). We differentiate two possibilities depending on the relative value of W and AS . In the case $W \gg AS$ we have a wide-band semiconductor (e.g. *EuTe*). In the opposite case $W \ll AS$, we talk about a “double-exchange” material (e.g. lanthanum manganites). For the sake of definiteness the sign of A is assumed to be positive. We also consider only the case $H = 0$ because at least up to fields $H \leq 2J$ (the field at which both sublattices collapse) the difference in energy for FM and AF parts always favored the conduction electron being in the FM part.

3 Variational procedure

As in references [1, 2, 3] a variational procedure will be used here to find the ground state energy of the phase-separated system. Three variational parameters are used, the ratio x of the volumes of the antiferromagnetic and ferromagnetic phases, the radius R of the spheres which form the multiply connected phase and $y = (N_F - N_A)/(N_F + N_A)$, where N_F (N_A) are the number of conduction electrons in the FM (AF) phase. y gives the ratio between the excess of electrons in a given phase and the total number of electrons and varies from -1 (all the electrons in the AF phase) to $+1$ (all the electrons in the FM phase).

With these definitions the densities of conduction electrons in each phase are:

$$\begin{aligned} n_F &= \frac{N_F}{V_F} = n(1+x) \frac{1+y}{2} \\ n_A &= \frac{N_A}{V_A} = n \left(\frac{1+x}{x} \right) \frac{1-y}{2} \end{aligned} \quad (2)$$

where n is the mean electron density in the crystal.

The trial energy is given by the expression:

$$E_{ps} = E_{kin} + E_{sur} + E_C + E_{mag} \quad (3)$$

where E_{kin} is the standard bulk kinetic energy of the conduction electrons, E_{sur} is the surface electron energy, i.e. the correction to E_{kin} that appears due to the quantization of the electron motion in regions of finite dimensions (in fact, this energy takes into account the electron level spatial quatization in a bounded region in the Born-Oppenheimer approximation), E_C is the electrostatic energy due to the inhomogeneous electronic density and E_{mag} is the magnetic energy. E_{mag} is decomposed in two parts: the energy associated to the s-d exchange interaction, E_{s-d} and the one associated to d-d exchange interaction, E_{d-d} .

We calculate now these energies for the phase-separated and the homogeneous states. As discussed in the introduction, we expect two different topologies of the phase-separated state depending on the conduction electron concentration. The conduction electron density at which this change occurs is denoted by n_T . Therefore we divide our calculation for the energy of the phase-separated state in the $n_d < n < n_T$ and $n_T < n < n_u$ cases. As we only consider here conduction electron concentrations over the $n_d < n < n_u$ range and magnetic fields smaller than the saturation field of

the material, the only possible homogeneous state we have to consider is the AF one. All the energies are calculated per unit volume of the unit cell and the numerical values are given in eV.

3.1 Energy of the phase separated state for $n_d < n < n_T$

Over this concentration range the phase-separated state is expected to be an AF matrix in which FM spheres are embedded. The total kinetic energy per unit volume of the unit cell is:

$$E_{\text{kin}} = \frac{E_{\text{kin}}^{\text{F}}}{1+x} + \frac{x E_{\text{kin}}^{\text{A}}}{1+x} \quad (4)$$

where $E_{\text{kin}}^{\text{F}}$ ($E_{\text{kin}}^{\text{A}}$) represent the energies of the conduction electrons in the FM (AF) phase.

In the ferromagnetic phase all the charge carriers are assumed to be spin-polarized. For $W \ll AS$ this condition is met for all the charge carrier densities. For $W \gg AS$ it is met when $AS > \mu$ where μ is their Fermi energy. It is also necessary to take into account the different band bottoms encountered by the charge carriers moving in the FM and the AF part of the crystal [5]. Therefore, in the free electron approximation, the kinetic energy of the conduction electrons in the FM phase is:

$$E_{\text{kin}}^{\text{F}} = -6tn_{\text{F}} + \frac{3}{5} \frac{(6\pi^2 n_{\text{F}})^{\frac{2}{3}}}{2m^* a^2} n_{\text{F}} \quad (5)$$

From now on $t = \frac{1}{2m^* a^2}$ and $\mu(n) = t(6\pi^2 n)^{\frac{2}{3}}$. Then:

$$E_{\text{kin}}^{\text{F}} = -6tn(1+x) \frac{1+y}{2} + \frac{3}{5} \mu(n)n(1+x)^{\frac{2}{3}} \left(\frac{1+y}{2} \right)^{\frac{5}{3}} \quad (6)$$

The kinetic energy of the conduction electrons in the antiferromagnetic part is:

$$E_{\text{kin}}^{\text{A}} = \begin{cases} -6tn \frac{1+x}{x} \frac{1-y}{2} + \frac{3}{5} 2^{-\frac{2}{3}} \mu(n)n \left(\frac{1+x}{x} \right)^{\frac{2}{3}} \left(\frac{1-y}{2} \right)^{\frac{5}{3}} & \text{if } W \gg AS \\ -\frac{6tn}{\sqrt{2S+1}} \frac{1+x}{x} \frac{1-y}{2} + \frac{3}{5} \frac{\mu(n)n}{\sqrt{2S+1}} \left(\frac{1+x}{x} \right)^{\frac{2}{3}} \left(\frac{1-y}{2} \right)^{\frac{5}{3}} & \text{if } W \ll AS \end{cases} \quad (7)$$

The surface energy, E_{sur} , appears due to the fact that the conduction electrons are confined in a finite volume. For each phase, it is proportional to $\frac{S}{V_i}$, being S the surface between both phases and V_i the volume of each phase, FM, V_{F} or AF, V_{A} respectively. We must point out that actually no surface energy independent of the conduction electron density can appear, because this term turns out meaningless in the case of the conduction electron density

equals to zero [1], where phase separation does not exist. The contribution to the surface energy due to magnetic interactions is also zero in the first-neighbour approximation considered by us.

$$E_{\text{sur}} = \frac{E_{\text{sur}}^{\text{F}}}{1+x} + \frac{x E_{\text{sur}}^{\text{A}}}{1+x} \quad (8)$$

where $E_{\text{sur}}^{\text{F}}$ ($E_{\text{sur}}^{\text{A}}$) represent the surface energies of the conduction electrons in the FM (AF) phase.

Taking into account the results of [6], we have in the FM part:

$$E_{\text{sur}}^{\text{F}} = \frac{5}{16} \left(\frac{\pi}{6} \right)^{\frac{1}{3}} \frac{S}{V_{\text{F}}} \frac{E_{\text{kin}}^{\text{F}}}{n_{\text{F}}^{\frac{1}{3}}} \quad (9)$$

Using the fact that $\frac{S}{V_{\text{F}}} = \frac{3}{R}$ being R (in a units) the radius of the ferromagnetic spheres containing the conduction electrons, we obtain:

$$E_{\text{sur}}^{\text{F}} = \frac{9}{16} \left(\frac{\pi}{6} \right)^{\frac{1}{3}} \frac{1}{R} \mu(n) n^{\frac{2}{3}} (1+x)^{\frac{1}{3}} \left(\frac{1+y}{2} \right)^{\frac{4}{3}} \quad (10)$$

For the AF part and making the obvious substitution in equation (10), we have:

$$E_{\text{sur}}^{\text{A}} = \begin{cases} \frac{9}{16} \left(\frac{\pi}{6} \right)^{\frac{1}{3}} \frac{1}{R} 2^{-\frac{2}{3}} \mu(n) n^{\frac{2}{3}} \left(\frac{1+x}{x^4} \right)^{\frac{1}{3}} \left(\frac{1-y}{2} \right)^{\frac{4}{3}} & \text{if } W \gg AS \\ \frac{9}{16} \left(\frac{\pi}{6} \right)^{\frac{1}{3}} \frac{1}{R} \frac{\mu(n) n^{\frac{2}{3}}}{\sqrt{2S+1}} \left(\frac{1+x}{x^4} \right)^{\frac{1}{3}} \left(\frac{1-y}{2} \right)^{\frac{4}{3}} & \text{if } W \ll AS \end{cases} \quad (11)$$

The Coulomb energy E_{C} is calculated using the jellium model for the ionized impurities. The crystal is separated into the Wigner cells, i.e. into spheres enveloping the FM inclusions drawn so as to make the total charge inside the sphere vanish. This method provides a good approximation to the electrostatic energy for small FM volumes, i.e. in the limit $x \gg 1$. Moreover it supposes to admit that the crystal is isotropic and homogeneous regarding the spatial distribution of these spheres. So we cannot describe the fractal nature of the boundary that separates phases. In this approximation:

$$E_{\text{C}} = \frac{2\pi}{5\epsilon_r} \frac{e^2 n^2 R^2}{x^2 a} \left(\frac{1-y}{2} - x \frac{1+y}{2} \right)^2 (2 + 3x - 3x^{\frac{1}{3}} (1+x)^{\frac{2}{3}}) \quad (12)$$

As was said above, the magnetic energy has two contributions. One part correspond to the antiferromagnetic interaction between the ionic d-shells, $E_{\text{d-d}}$. We estimate it within the mean field approximation. Because our

calculation is constrained to $T = 0$, we only have to take into account the ground state of the system. For the antiferromagnetic phase we have:

$$E_{d-d}^A = -\frac{|J|S}{2} \quad (13)$$

where $|J| = -\frac{zIS}{2}$. For the ferromagnetic phase:

$$E_{d-d}^F = \frac{|J|S}{2} \quad (14)$$

Therefore the total energy E_{d-d} is:

$$E_{d-d} = \frac{x E_{d-d}^A}{1+x} + \frac{E_{d-d}^F}{1+x} = \frac{|J|S}{2} \frac{1-x}{1+x} \quad (15)$$

We assume that the AF part is in an collinear AF state. A canted AF state would be also possible. In the case a fourth parameter, namely the canting angle, must be added to the minimization procedure. Its value depends only on the conduction electron density, which in the AF part of the phase-separated state depends on the parameters x, y . We ruled out this possibility in the view of the results in reference [7] where it is shown that the canted state is unstable against charge-carrier density fluctuations and it is never realized. The second part corresponds to the energy due to the interaction between the conduction electrons and magnetic ions, E_{s-d} . Again we have:

$$E_{s-d} = \frac{x E_{s-d}^A}{1+x} + \frac{E_{s-d}^F}{1+x} \quad (16)$$

where in the FM part:

$$E_{s-d}^F = -\frac{AS}{2} n_F = -\frac{AS}{2} n(1+x) \frac{1+y}{2} \quad (17)$$

And in the AF part:

$$E_{s-d}^A = \begin{cases} 0 & \text{if } W \gg AS \\ -\frac{AS}{2} n \frac{1+x}{x} \frac{1-y}{2} & \text{if } W \ll AS \end{cases} \quad (18)$$

Notice that for $W \ll AS$, A does not appears in the calculation, it is only an additive constant.

3.2 Energy of the phase-separated state for $n_T < n < n_u$

In the case of that the density of the conduction electrons is higher than the percolation density n_T , a phase transition is expected with a change in the sample topology. The sample changes from being a AF matrix in which FM spheres are embedded to have a simply connected FM part with AF spheres in. To take this point into account we have to modify surface and Coulomb energies as follows:

$$\begin{aligned}
E_C &= \frac{2\pi}{5\epsilon_r} \frac{e^2 n^2 R^2 x}{a} \left(\frac{1+y}{2x} - \frac{1-y}{2} \right)^2 (2 + 3x - 3x^{\frac{1}{3}}(1+x)^{\frac{2}{3}}) \\
E_{\text{sur}}^F &= \frac{9}{16} \left(\frac{\pi}{6} \right)^{\frac{1}{3}} \frac{1}{R} \mu(n) n^{\frac{2}{3}} x (1+x)^{\frac{1}{3}} \left(\frac{1+y}{2} \right)^{\frac{4}{3}} \\
E_{\text{sur}}^A &= \begin{cases} \frac{9}{16} \left(\frac{\pi}{6} \right)^{\frac{1}{3}} \frac{1}{R} 2^{-\frac{2}{3}} \mu(n) n^{\frac{2}{3}} \left(\frac{1+x}{x} \right)^{\frac{1}{3}} \left(\frac{1-y}{2} \right)^{\frac{4}{3}} & \text{if } W \gg AS \\ \frac{9}{16} \left(\frac{\pi}{6} \right)^{\frac{1}{3}} \frac{1}{R} \frac{\mu(n) n^{\frac{2}{3}}}{\sqrt{2S+1}} \left(\frac{1+x}{x} \right)^{\frac{1}{3}} \left(\frac{1-y}{2} \right)^{\frac{4}{3}} & \text{if } W \ll AS \end{cases}
\end{aligned} \tag{19}$$

The others energies remain unchanged.

3.3 Energy of the homogeneous phase

Over the concentration range $n_d < n < n_u$ the homogeneous antiferromagnetic phase has an energy:

$$E_{\text{hom}} = E_{\text{kin}}^{\text{hom}} + E_{\text{mag}}^{\text{hom}} \tag{20}$$

where

$$E_{\text{kin}}^{\text{hom}} = -6tn + \frac{3}{5} 2^{-\frac{2}{3}} \mu(n) n \quad E_{\text{mag}}^{\text{hom}} = -\frac{|J|S}{2} \tag{21}$$

if $W \gg AS$ and

$$E_{\text{kin}}^{\text{hom}} = -\frac{6tn}{\sqrt{2S+1}} + \frac{3}{5} \frac{\mu(n)n}{\sqrt{2S+1}} \quad E_{\text{mag}}^{\text{hom}} = -\frac{|J|S}{2} - \frac{ASn}{2} \tag{22}$$

if $W \ll AS$

4 Results

The stationary state of the system is determined from the condition that the total energy of the system equation (3) be a minimum with respect to the

three variational parameters x , R and y . The parameter R only appears in the surface and Coulomb energies. Minimizing the sum $Q = E_{\text{sur}} + E_{\text{C}}$ with respect to R for fixed x and y leads to the following expressions:

$$\begin{aligned} Q_{\min} &= \alpha\gamma(hfg^2)^{\frac{1}{3}} \\ R_{\min} &= \alpha'\gamma'\left(\frac{g(x,y)}{h(x,y)f(x)}\right)^{\frac{1}{3}} \end{aligned} \quad (23)$$

where:

$$\begin{aligned} \alpha &= 3\left(\frac{2\pi}{5}\right)^{\frac{1}{3}}\left(\frac{9}{32}\right)^{\frac{2}{3}}\left(\frac{\pi}{6}\right)^{\frac{2}{9}} \approx 1.2 & \gamma &= \left(\frac{n^{\frac{1}{3}}e^2}{\epsilon_r a}\mu^2 n\right)^{\frac{1}{3}} \\ \alpha' &= \left(\frac{\frac{9}{32}\left(\frac{\pi}{6}\right)^{\frac{1}{6}}}{\frac{2\pi}{5}}\right)^{\frac{1}{3}} \approx 0.59 & \gamma' &= \left(\frac{\mu(n)n^{-\frac{4}{3}}}{\frac{e^2}{\epsilon_r a}}\right)^{\frac{1}{3}} \end{aligned}$$

We have used the following definitions:

$$\begin{aligned} f(x) &= 2x + 3 - 3(1+x)^{\frac{2}{3}} \\ g(x,y) &= \left(\frac{1+y}{2}\right)^{\frac{4}{3}}(1+x)^{\frac{1}{3}} + \chi\left(\frac{1-y}{2}\right)^{\frac{4}{3}}\left(\frac{1+x}{x^4}\right)^{\frac{1}{3}} \\ h(x,y) &= \frac{1}{x^2}\left(\frac{1-y}{2} - x\frac{1+y}{2}\right)^2 \end{aligned} \quad (24)$$

if $n_{\text{d}} < n < n_{\text{T}}$.

In the case of a multiply connected AF phase, i.e. for $n_{\text{T}} < n < n_{\text{u}}$, the latter expressions are modified according to:

$$\begin{aligned} f(x) &= 2 + 3x - 3x^{\frac{1}{3}}(1+x)^{\frac{2}{3}} \\ g(x,y) &= \left(\frac{1+y}{2}\right)^{\frac{4}{3}}x(1+x)^{\frac{1}{3}} + \chi\left(\frac{1-y}{2}\right)^{\frac{4}{3}}\left(\frac{1+x}{x}\right)^{\frac{1}{3}} \\ h(x,y) &= x\left(\frac{1+y}{2x} - \frac{1-y}{2}\right)^2 \end{aligned} \quad (25)$$

In both cases we have introduced the parameter χ equal to $2^{-\frac{2}{3}}$ if $W \gg AS$ and to $(2S+1)^{-\frac{1}{2}}$ if $W \ll AS$.

After substituting equation (23) into equation (3) minimization with respect to x and y is carried out numerically.

The percolation density n_{T} is calculated by solving for the value of n at which both separate phases are minimal as a function of x and y and have

the same energy. For n_d and n_u , the requirements are that the separate state have a minimum as a function of x , and its energy being equal to that of the corresponding homogeneous state¹.

The values of the parameters that characterize wide-band semiconductors are chosen the same as in reference [4] (they correspond to rare-earth compounds of the *EuTe* type): $S = \frac{7}{2}$, $|J|S = 10^{-3}$ eV (that implies $T_N = 5$ K, and the field at which both sublattices collapse is 98.7 kOe), $AS = 1$ eV, $\epsilon_r = 20$, $a^{-3} = 4 \cdot 10^{22}$ cm⁻³, and the electron effective mass is equal to free electron mass, this implies $W = 4$ eV. The value obtained for $n_T = 1.10 \cdot 10^{20}$ cm⁻³. The value for n_u , at which the conductive phase-separated state becomes unstable at $H = T = 0$ is $1.79 \cdot 10^{20}$ cm⁻³. In this work we consider the following electron concentrations $0.9 n_T$ and $1.3 n_T$, as an example of both topologies. To study the difference in energies between the energy of the homogeneous antiferromagnetic phase E_{hom} and the energy of the phase-separated state E_{ps} for both electron concentrations we show in figures 1 and 2 a contour plot of the energy difference $\Delta E = \frac{E_{\text{ps}} - E_{\text{hom}} - |E_{\text{ps}} - E_{\text{hom}}|}{2n}$ as a function of x and y . Notice that $\Delta E = 0$ if $E_{\text{ps}} \geq E_{\text{hom}}$. The lines on the diagram are lines of constant ΔE . The regions with no lines correspond to $\Delta E = 0$. The lines in the upper part of the figures correspond to more negative energy differences. It can be observed that as y increases ΔE becomes more negative. In both cases, the minimum value of ΔE is obtained for $y = 1$, i.e. $N_A = 0$. For the values of n we show here, the minima are $\frac{E_{\text{ps}} - E_{\text{hom}}}{n}(x = 1.3662, y = 1) = -0.1707$ at $n = 0.9 n_T$ and $\frac{E_{\text{ps}} - E_{\text{hom}}}{n}(x = 0.5169, y = 1) = -0.2095$ at $n = 1.3 n_T$.

The values of parameters that characterize “double-exchange” semiconductors are the following (typical for lanthanum manganites, for example): $S = 2$, $D = -zIS^2 = 10^{-2}$ eV (that implies $T_N = 58$ K, and the field at which the two sublattices collapse at $T = 0$ is 1.73 MOe), $\epsilon_r = 5$, $a^{-3} = 4 \cdot 10^{22}$ cm⁻³, the effective electron mass equal to the free electron mass, that implies $W = 4$ eV. A is regarded as high enough to meet $W \ll AS$, although its precise value is not needed for calculation. We obtain $n_T = 5.93 \cdot 10^{20}$ cm⁻³ and $n_u = 9.46 \cdot 10^{20}$ cm⁻³. As before we consider the following electron concentrations $0.9 n_T$ and $1.3 n_T$. The energy minima are $\frac{E_{\text{ps}} - E_{\text{hom}}}{n}(x = 1.3159, y = 1) = -0.04454$ at $n = 0.9 n_T$ and $\frac{E_{\text{ps}} - E_{\text{hom}}}{n}(x = 0.4681, y = 1) = -0.1162$ at $n = 1.3 n_T$. Contour plots are shown in figures 3 and 4. In both cases minima are found in $y = 1$, i.e. all the conduction electrons are in the AF part of the phase-separated states.

Analogous results are obtained for any value of the concentration of conduction electrons over the range $n_d < n < n_u$. Therefore, we have shown that

¹Our values for n_T are slightly different from those in [5], calculated imposing $x = y = 1$.

for both kinds of compounds and over the above mentioned range of concentrations, the ground state corresponds to a phase-separated state with FM and AF parts, with absence of electrons in the antiferromagnetic part.

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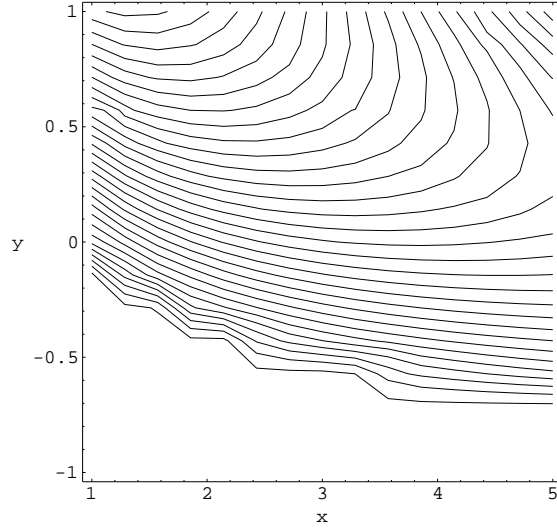


Figure 1: Countour plot of ΔE as a funtion of x, y for $W \gg AS$ and $n = 0.9n_T$. Lines in the upper part correspond to more negative ΔE .

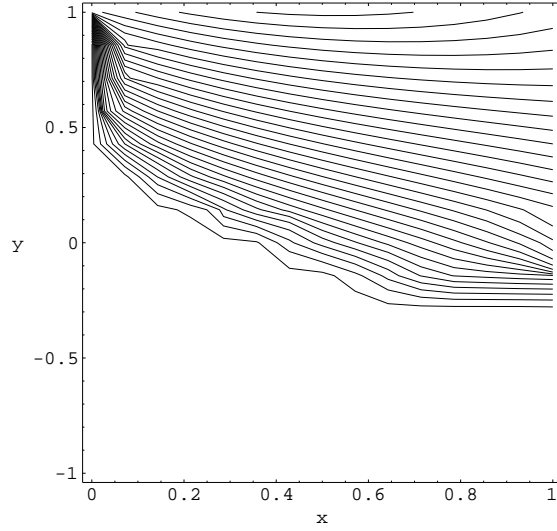


Figure 2: Countour plot of ΔE as a funtion of x, y for $W \gg AS$ and $n = 1.3n_T$. Lines in the upper part correspond to more negative ΔE .

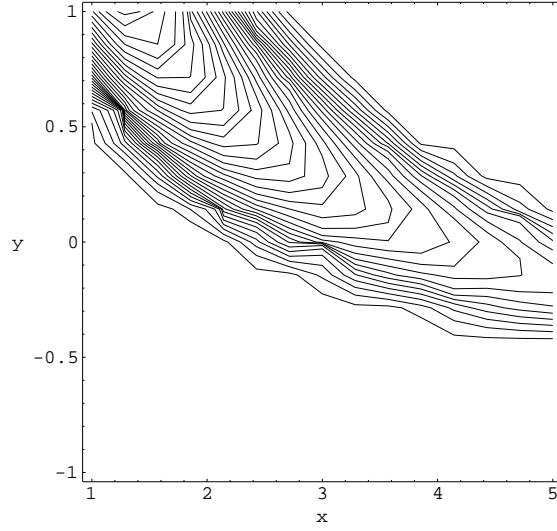


Figure 3: Countour plot of ΔE as a funtion of x, y for $W \ll AS$ and $n = 0.9n_T$ Lines in the upper part correspond to more negative ΔE .

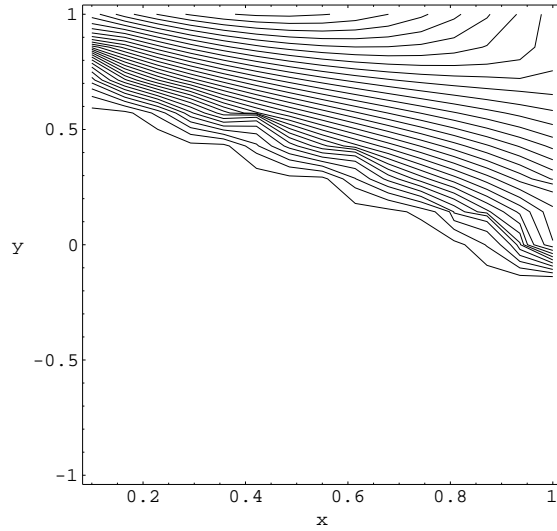


Figure 4: Countour plot of ΔE as a funtion of x, y for $W \ll AS$ and $n = 1.3n_T$ Lines in the upper part correspond to more negative ΔE .